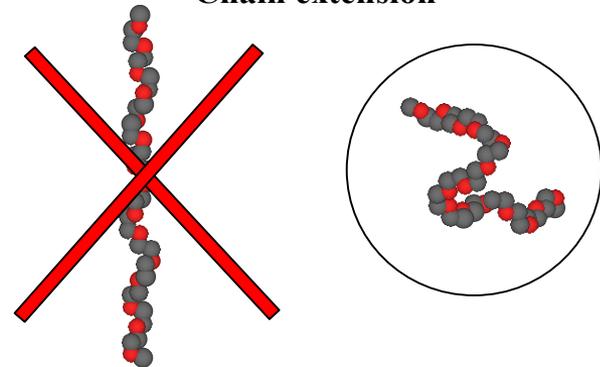
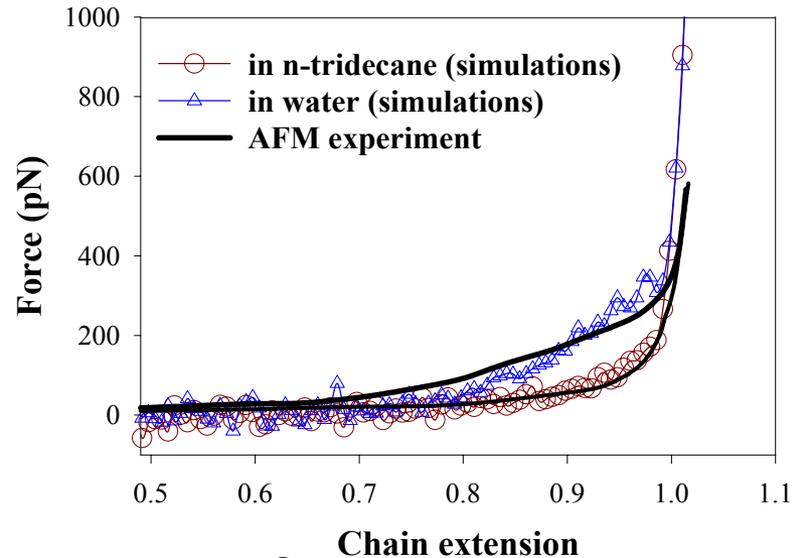


Poly(ethylene oxide) and Water: Simulations and Modeling of Solution Properties, Phase Behavior, Partitioning and Particle Interactions

Grant D. Smith, University of Utah, DMR-0076306

The conformations of poly(ethylene oxide) (PEO) in aqueous solution are largely responsible for the properties of these solutions that have resulted in the use of PEO in applications ranging from protein crystallization to drug delivery. Despite their importance, the conformations of PEO in water remain controversial. Based mainly upon an increase in the gauche population of O-C-C-O dihedrals observed spectroscopically, it has been surmised that PEO adopts a helical conformation in water that is commensurate with the structure of liquid water. Recently, the restoring force observed in stretching of a single PEO chain in aqueous solution via atomic force microscopy (AFM) have also been interpreted in terms of helical conformations. Our molecular dynamics (MD) simulations of PEO in water yield a restoring force vs. chain extension in quantitative agreement with these experiments. Detailed analysis of MD simulations of PEO solutions show no tendency for formation of helical PEO conformations in water or in non-polar alkane solvents.



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Education:

This project has resulted in two Ph.D.'s (Dmitry Bedrov, Oleg Borodin) and one Master's Degree (Richard Douglas). Three undergraduate students (Richard Douglas, Lora Lee Wirth and Mike Fuller) were also supported on this project. Force field development for PEO/water solutions supported by this project formed the core of the P.I.'s contribution to the American Physical Society, Division of Polymer Physics, short course on "Molecular Simulations of Polymers", presented in Seattle, March 2001.

Outreach:

Graduate students, undergraduate students and the P.I. actively participate in annual the MSE Open House as well as the spring and fall Engineering Week at the University of Utah. These events are designed to expose junior high and high school students with interest in science and engineering to engineering, and to attract these students to MSE. The photo shows the Molecular Modeling Exhibit largely designed and constructed by graduate and undergraduate students supported by NSF.

